CLAIMS

1. Isopenicillin N synthase (IPNS) in the form of: a complex with Fe and its substrate, said complex having a structure substantially designated by the X-ray co-ordinates in Table 3.

2. The IPNS complex of claim 1, wherein the substrate is L-δ-α-aminoadipoyl-L-cysteinyl-D-valine (ACV).

3. The IPNS complex of claim 1 wherein the substrate is an analogue of ACV selected from AC glycine, Ac aminobutyrate, AC alanine and AC propargylglycine.

4. Use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.

5. Use as claimed in claim 4, wherein the second enzyme is modified: to accept unnatural substrates for the preparation of antibacterial materials or intermediate for the production of pharmaceutical products; or to produce unnatural products or improve the production of natural products.

6. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

N287; R87; A88; Y189; S183; Y91; F285; Q330; T331; V185; L106; C104; V217; L324; L317; I325; L321; S210.

7. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

V272; L231; L223; P283; T221; F211, F285; Q330; I187; V185; Y189; R279; S281; N230; Q225; N252; S210.

8. A gene which codes for the enzyme of claim 6 or claim 7.

9. A micro-organism containing the gene of claim 8 and which is capable of expressing the gene under fermentation conditions.

10. Use of the micro-organism of claim 9 for making a bicyclic β-lactam of the penicillin or cephalosporin (including cephams) families.

11. Use of the enzyme of claim 6 or claim 7 for the preparation *in vitro* of a bicyclic β-lactam of the penicillin or cephalosporin families.

12. In a method for the preparation of an enzyme, selected from IPNS, DAOCS, DACS, DAOC/DACS and sequence-related enzymes, in crystalline form for X-ray diffraction studies, the improvement which consists in maintaining the enzyme under anaerobic conditions with dioxygen substantially absent.

13. A method which comprises using the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for determining or predicting the structure of a second enzyme which is structurally related to the first enzyme but is not active in the penicillin or cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the second enzyme or for designing an inhibitor for the second enzyme.

14. Use of the enzyme of claim 6 or claim 7 to convert a dipeptide to a 6- aminopenicillin or other bicyclic β-lactam.

15. Use as claimed in claim 14, wherein the dipeptide has been produced by use of a peptide synthetase enzyme such as L-δ-α-aminoadipoyl-L-cysteinyl-D-valine (ACV) synthetase optionally modified to optimise dipeptide production.